Sandia National Laboratories

Environmental Program

Geochemistry Department

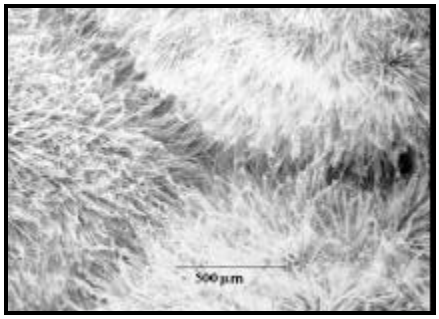
Focus

The Geochemistry Department's applied and basic research or support activities are directed at a broad range of topics, including: standard geochemical characterization of rocks and fluids, natural weathering reactions, ion exchange mechanisms, sorption and desorption kinetics, transport and attenuation processes for toxic metal and radionuclide species, computer modeling of reactive fluid flow in fractured and porous media, theoretical modeling of bulk and interfacial mineral-fluid processes using ab initio and empirical techniques, and development of waste site remediation techniques. The Geochemistry Department supports a variety of analytical, experimental, and theoretical projects, including:

- Characterization of silicate mineral dissolution, precipitation & growth kinetics and reaction mechanisms.
- Empirical and ab initio modeling of complex mineral structures and mineral-solution interfaces, emphasizing sorption processes.
- In-situ waste remediation and attenuation studies, focusing on sorption, desorption and ion exchange mechanisms with common soil and rock surfaces.
- Calculation of mineral equilibria, stability phase diagrams and solution reaction paths for waste site and waste form performance assessment.
- Design and evaluation of repository backfills, including MgO, cement, clays, and radionuclide-specific getters.
- Identification of mechanistic processes that control metal and organic attenuation by irreversible sorption in the subsurface.
- High temperature and hydrothermal synthesis, reaction, and kinetic studies.
- Lattice Boltzmann computational modeling of mesoscale fluid flow and reaction in fractured and porous media.

Laboratory Facilities

Scanning electron microscope with energy-dispersive analyzer (C-U); High resolution automated X-ray diffractometer; Atomic Force Microscope for molecular scale topographic characterization of crystal surfaces; Ion selective electrodes and computer-controlled batch reaction titrators; Oxygen-controlled furnace for mineral synthesis and reaction (<1700°C); Ion chromatograph (IC) with gradient eluent pump and direct current plasma spectrometer for analyis of liquids; Cold-seal and Dickson pressure vessels for hydrothermal synthesis or reaction (up to 100 MPa and 800°C); Light element stable isotope mass spectrometers; Karl-Fischer water analyzer; Infrared and ultraviolet/visible spectrometers; Geologic and petrographic sample preparation laboratory.



MgO pellets reacted in WIPP brine to form strength-enhancing Sorel cement

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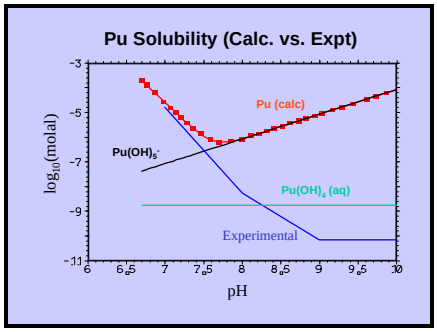
(http://www.sandia.gov/eesector/gs/gc/geochem.html)

Computer Modeling Capabilities

Two codes, **EQ3/6** and **Geochemist's Workbench**, contain internally consistent thermodynamic databases for minerals, aqueous species, and gases and are used to predict fluid-rock interactions, mineral stabilities and solid solution assemblages as a function of temperature, pressure and time. **Molecular Simulations Inc. Catalysis and Sorption** software is an integrated suite of commercial grade computer programs for the simulation of molecular dynamics, lattice energy, and approximate molecular orbital simulations of organic and inorganic systems. **Lattice Gas Automata and Lattice Boltzmann** codes are used to calculate flow, transport and reaction of solutes and immiscible liquids for such diverse processes as tracer dispersion and retardation in porous media and fracture flow.



Solubility of Pu° and dissolved Pu-species

Selected Projects

Characterization of Retardation Mechanisms in Soils: Experimental, spectroscopic, and theoretical studies of mineral-solution interfaces and the sorption of alkali and alkaline earth metals onto simple oxyhydroxide and layered silicate structures (sponsor: Nuclear Regulatory Commission)

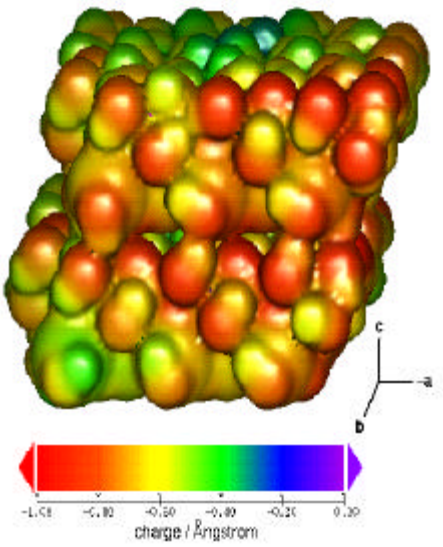
Phase Chemistry of Tank Sludge Residual Components: Analytical and experimental study of radioactive tank waste phases and development of a scientifically defensible model describing the export of radiotoxicity from radwaste storage tanks (sponsor: Environmental Management Science Program)

Cation Diffusion Rates in Selected Minerals: *Carbonates, Garnets, and Pyroxenes*: Experimental studies and modeling of cation diffusion in carbonate and silicate minerals at elevated temperatures, and theoretical analysis of diffusion mechanisms and point defect structure (sponsor: Office of Basic Energy Science/Geosciences)

An Investigation of Organic Anion-Mineral Surface Interactions During Diagenesis: Experimental measurement and computer modeling of organic anion adsorption to mineral surfaces to understand geochemical controls on diagenesis and weathering of soil silicate minerals (sponsor: Office of Basic Energy Science/Geosciences)

Doping of Lithium Manganese Oxide for Improved Battery Performance: Theoretical empirical modeling of the structure and lattice energies of doped lithium manganese oxide structures, including calculation of the diffusion of Li ions in spinel (sponsor: Office of Basic Energy Science/Chemical Sciences).

Development, Implementation, and Experimental Validation of the Lattice Boltzmann Method for Modeling Three-Dimensional Complex Flows: Lattice Boltzmann modeling of 3D mesoscale flow and reaction in porous media (sponsor: SNL Internal R&D (LDRD) Funding).

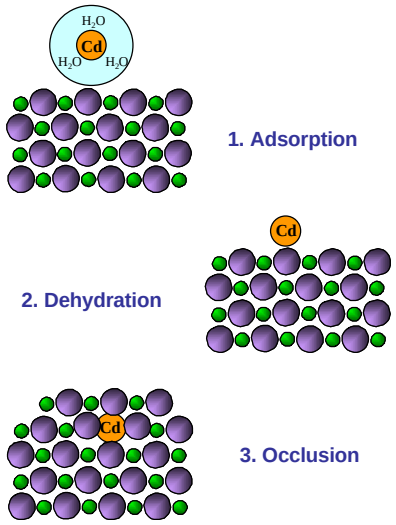


Molecular Electrostatic Potential Surface of (010) Kaolinite Clay

CO_2 Reactivity with MgO Backfill: Experimental and analytical characterization of the reactivity of MgO as a backfill in evaporite rock/brine environments and the development of thermally-accelerated testing procedures for characterizing the kinetics of these interactions (sponsor*:* Waste Isolation Pilot Plant).

Mechanistic Models for Radionuclide Desorption from Soils: The Sandia Natural Attenuation Project is an experimental, theoretical, and field program to identify the mechanistic controls on metal and organic attenuation by irreversible sorption in the subsurface. SNAP will provide a scientific basis for risk-based corrective actions by helping identify only those sites where contaminants can be expected to impact the biosphere (sponsor: SNL Internal R&D (LDRD) Funding).

Molecular Controls on Actinide Sorption: Experimental and theoretical studies of mineral-solution interfaces and dissolved complexes focussing on actinide speciation, and sorption onto dolomite (sponsor*:* Waste Isolation Pilot Plant).



Schematic of irreversible sorption for Cd on a mineral surface

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